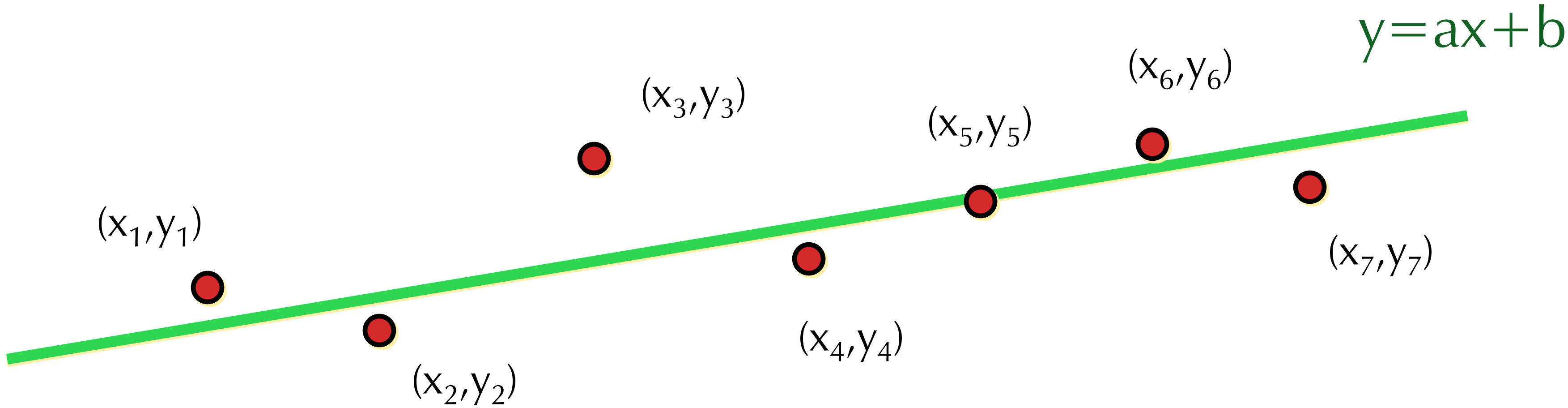
Data Modeling and Least Squares Fitting

COS 323

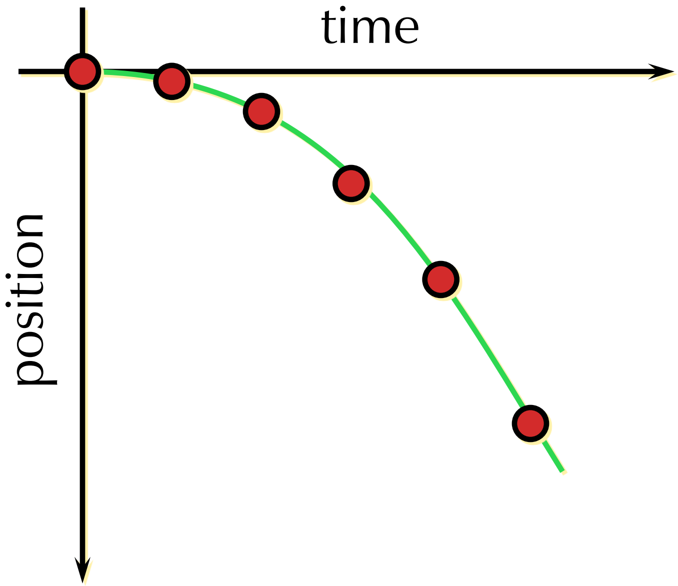
Data Modeling or Regression

- Given: data points, functional form, find constants in function
- Example: given (x_i, y_i), find line through them; i.e., find a and b in $y = ax+b$



Data Modeling

- You might do this because you actually care about those numbers…
  - Example: measure position of falling object, fit parabola

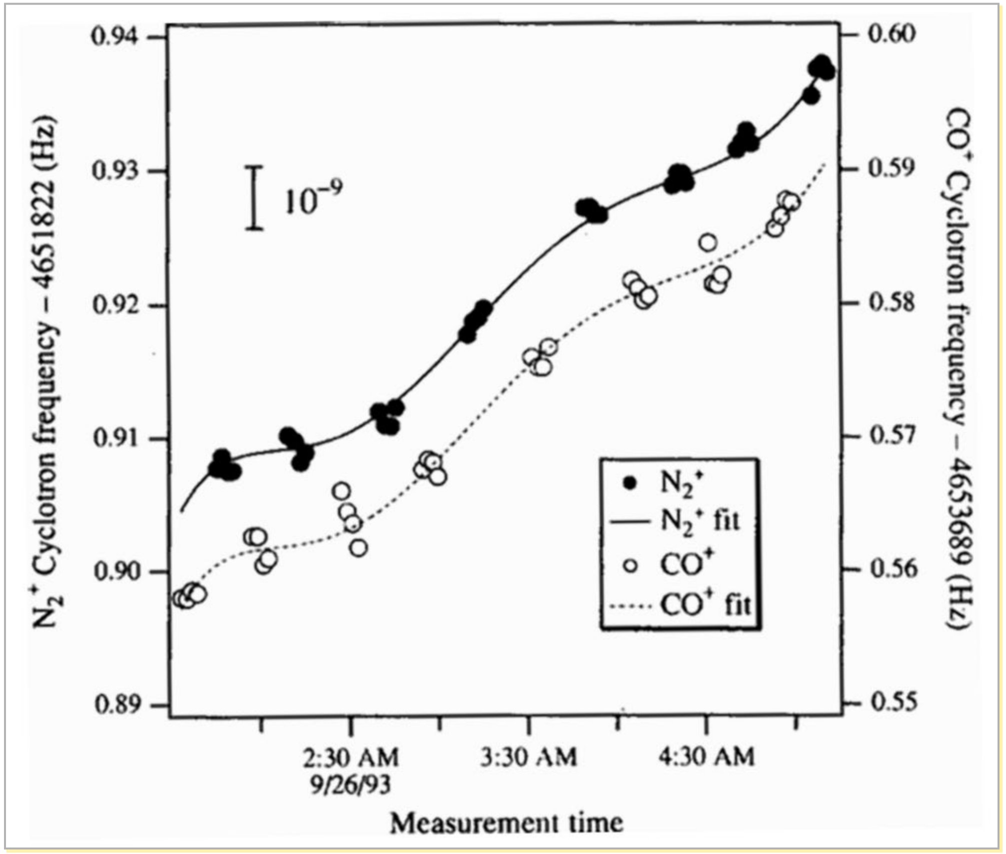


$z = -{}^{1}/_{2}\, g t^2$

data points (t_i, z_i) known
constant g unknown
$\Rightarrow$ Estimate g from fit

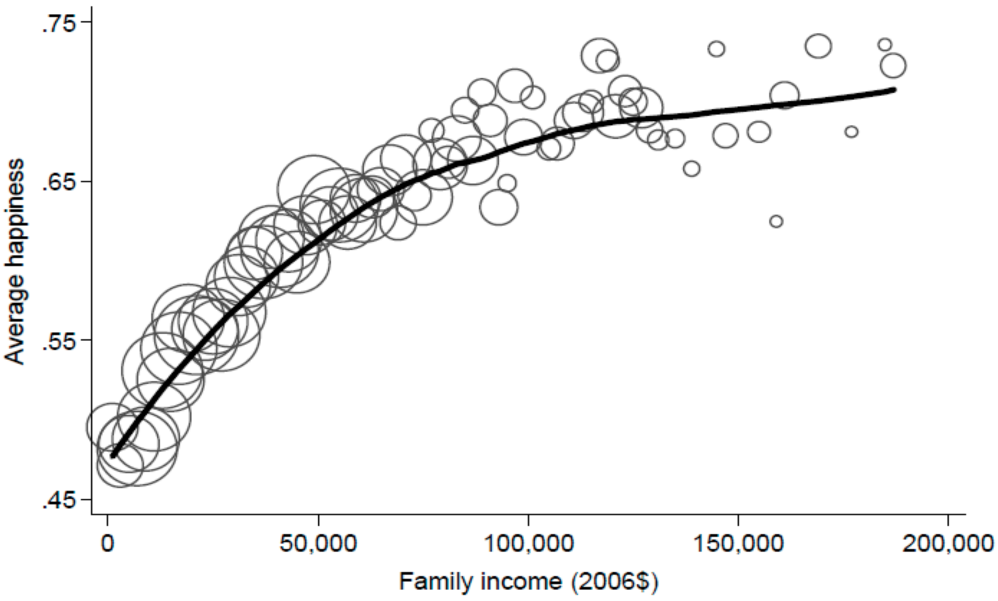
Data Modeling

- … or because some aspect of behavior is unknown and you want to ignore it
  - Measuring relative resonant frequency of two ions, want to ignore magnetic field drift



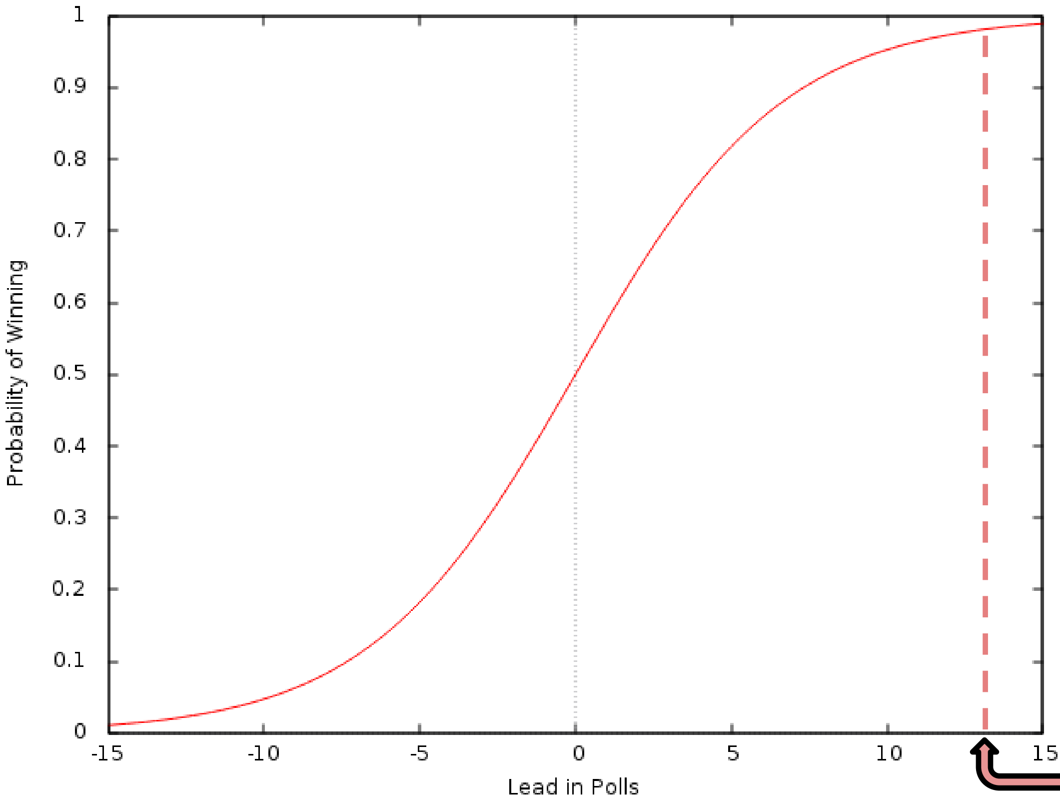
Data Modeling

- … or to compare model types to figure out what *kind* of dependence exists
  - Is happiness linear w.r.t. income?



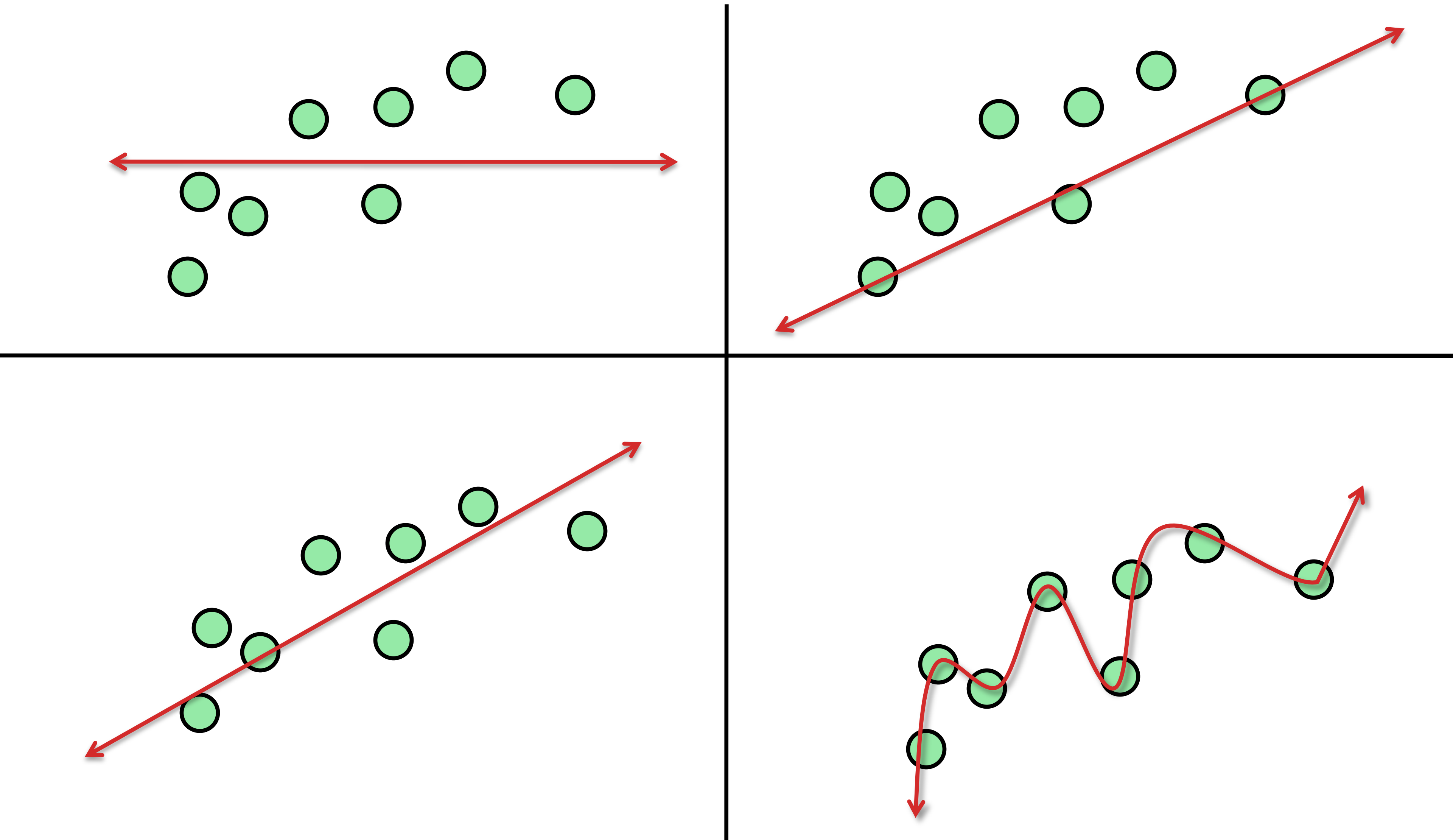
Data Modeling

- … or to make predictions

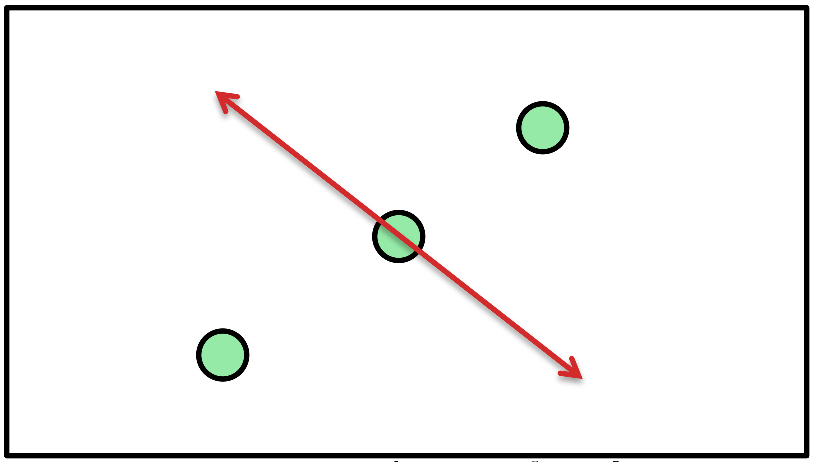


Corey Booker's current lead

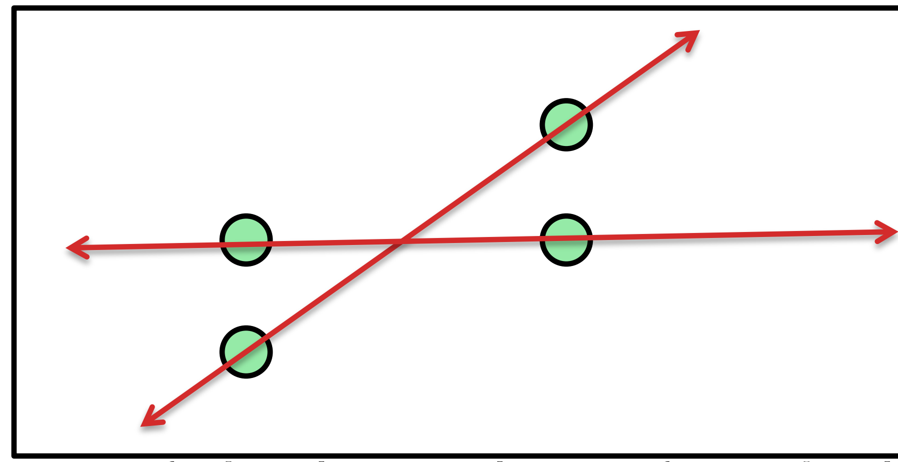
Which model is best?



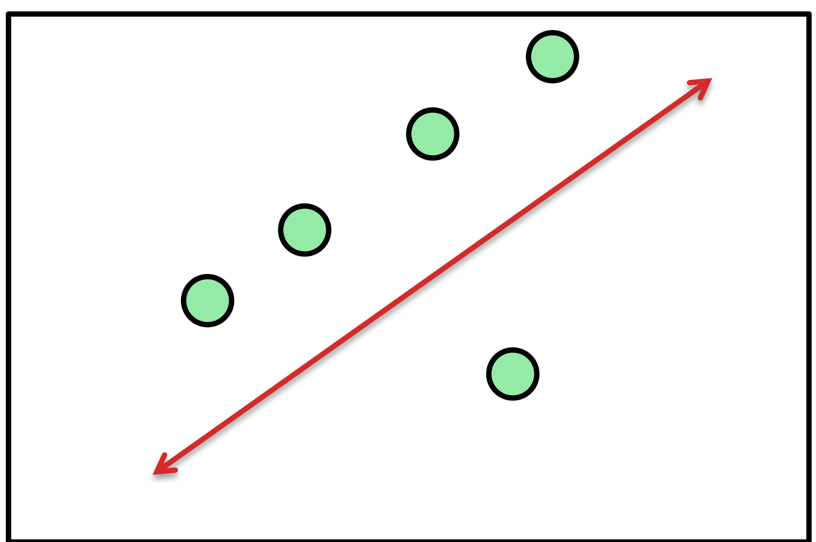
Best-fit lines under different metrics



Sum of residuals



Sum of absolute values of residuals



Maximum error of any point

Least Squares

- Nearly universal (but problematic!) formulation:

  minimize squares of differences
  between data and function

  – Example: to fit a line to points (x_i, y_i), minimize

$$\chi^2 = \sum_i \left(y_i - (ax_i + b)\right)^2$$

  with respect to a and b

Linear Least Squares

- Important special case
  - (Also called "Ordinary least squares")
- General pattern:

$$y_i = a\, f(\vec{x}_i) + b\, g(\vec{x}_i) + c\, h(\vec{x}_i) + \cdots$$

$$\text{Given } (\vec{x}_i, y_i), \text{ solve for } a, b, c, \ldots$$

- *Dependence on unknowns (a, b, c…)* is linear, but f, g, etc. might not be!

Linear Least Squares Examples

- General form: $y_i = a\,f(\vec{x}_i) + b\,g(\vec{x}_i) + c\,h(\vec{x}_i) + \cdots$

  Given $(\vec{x}_i, y_i)$, solve for $a, b, c, \ldots$

- **Linear** regression: $f(x_i) = x_i$, $g(x_i) = 1$

  $y_i = a * x_i + b$

- **Multiple** linear regression:

  $y_i = a * x_{1i} + b * x_{2i} + c$

- **Polynomial** regression:

  $y_i = a * x_i^2 + b * x_i + c$

Linear Least Squares Pros and Cons

+ Relatively simple to compute
+ Easy to analyze stability / adequacy of data
+ Given sufficient data, exactly one solution

– Sensitive to outliers
– Temptation to model nonlinear dependency as linear

How do we compute the model parameters?

Solving Linear Least Squares Problem (one simple approach)

- Take partial derivatives:

$$\chi^2 = \sum_i \left(y_i - a\, f(x_i) - b\, g(x_i) - \cdots \right)^2$$

$$\frac{\partial}{\partial a} = \sum_i -2 f(x_i) \left(y_i - a\, f(x_i) - b\, g(x_i) - \cdots \right) = 0$$

$$a \sum_i f(x_i) f(x_i) + b \sum_i f(x_i) g(x_i) + \cdots = \sum_i f(x_i)\, y_i$$

$$\frac{\partial}{\partial b} = \sum_i -2 g(x_i) \left(y_i - a\, f(x_i) - b\, g(x_i) - \cdots \right) = 0$$

$$a \sum_i g(x_i) f(x_i) + b \sum_i g(x_i) g(x_i) + \cdots = \sum_i g(x_i)\, y_i$$

Solving Linear Least Squares Problem

- For convenience, rewrite as matrix:

$$\begin{bmatrix} \sum_i f(x_i)f(x_i) & \sum_i f(x_i)g(x_i) & \cdots \\ \sum_i g(x_i)f(x_i) & \sum_i g(x_i)g(x_i) & \\ & \vdots & \end{bmatrix} \begin{bmatrix} a \\ b \\ \vdots \end{bmatrix} = \begin{bmatrix} \sum_i f(x_i)\, y_i \\ \sum_i g(x_i)\, y_i \\ \vdots \end{bmatrix}$$

- Factor:

$$\sum_i \begin{bmatrix} f(x_i) \\ g(x_i) \\ \vdots \end{bmatrix} \begin{bmatrix} f(x_i) \\ g(x_i) \\ \vdots \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} a \\ b \\ \vdots \end{bmatrix} = \sum_i y_i \begin{bmatrix} f(x_i) \\ g(x_i) \\ \vdots \end{bmatrix}$$

Alternative Perspective: Overconstrained (Approximate) Linear System

- There's a different derivation of this: overconstrained linear system

$$\mathbf{A}x = b$$

$$\begin{pmatrix} \\ \\ & \mathbf{A} & \\ \\ \\ \end{pmatrix} \begin{pmatrix} \\ x \\ \\ \end{pmatrix} = \begin{pmatrix} \\ \\ b \\ \\ \\ \end{pmatrix}$$

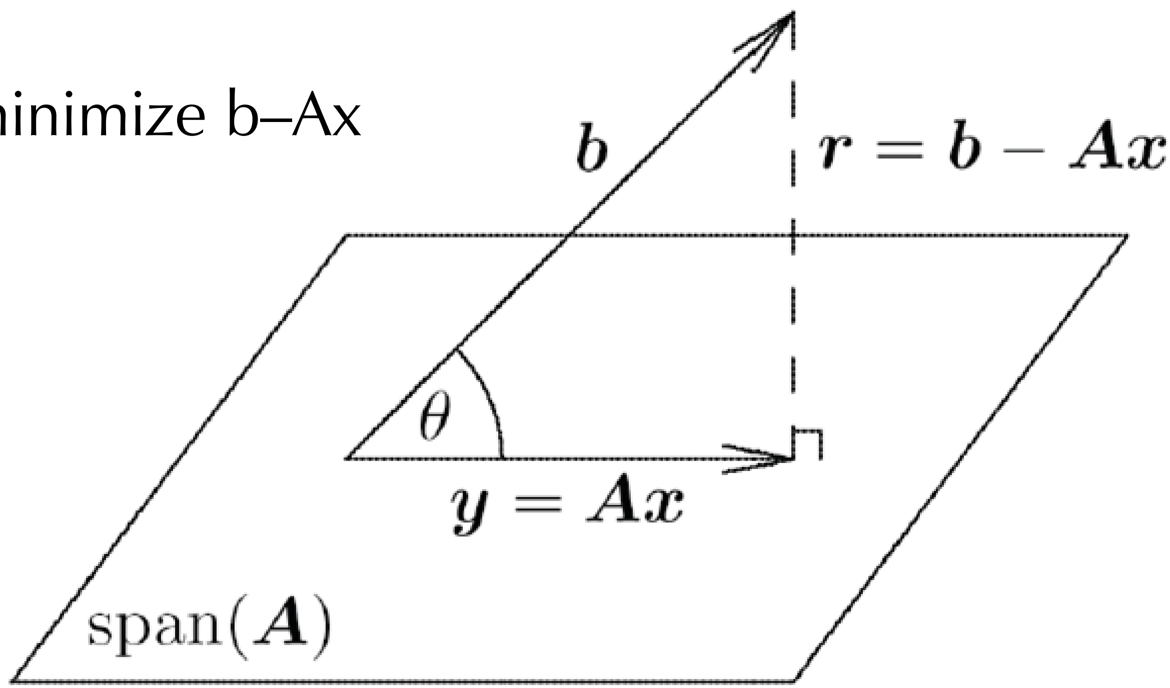
Notation:

- Rows of **A** are basis functions computed on observations ($f(x_i)$, $g(x_i)$, …)
- x is column of model parameters (a, b, c…)
- b is column of "y_i"

- **A** has n rows and m<n columns: more equations than unknowns

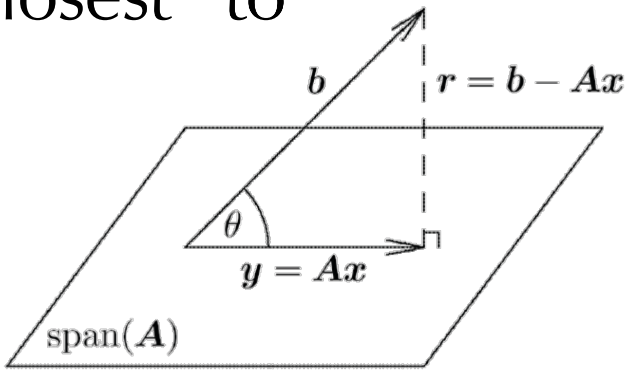
Geometric Interpretation for Over-determined System

- Find the x that comes "closest" to satisfying Ax=b
  - i.e., minimize b–Ax



Geometric Interpretation

- Interpretation: find x that comes "closest" to satisfying Ax=b
  - i.e., minimize b–Ax
  - i.e., minimize || b–Ax ||
  - Equivalently, find x such that r is orthogonal to span(A)



$$0 = \mathbf{A}^T\mathbf{r} = \mathbf{A}^T(\mathbf{b} - \mathbf{A}\mathbf{x})$$

$$\mathbf{A}^T\mathbf{A}\mathbf{x} = \mathbf{A}^T\mathbf{b}$$

Forming the equation

- What are A and b?
  - Row i of A is basis functions computed on x_i
  - Row i of b is y_i

$$\mathbf{A} = \begin{bmatrix} f(x_1) & g(x_1) & \cdots \\ f(x_2) & g(x_2) & \cdots \\ & \vdots & \end{bmatrix}, \quad b = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \end{bmatrix}$$

$$\mathbf{A}^{\mathrm{T}}\mathbf{A} = \begin{bmatrix} \sum_i f(x_i)f(x_i) & \sum_i f(x_i)g(x_i) & \cdots \\ \sum_i g(x_i)f(x_i) & \sum_i g(x_i)g(x_i) & \cdots \\ & \vdots & \end{bmatrix}, \quad \mathbf{A}^{\mathrm{T}}b = \begin{bmatrix} \sum_i y_i f(x_i) \\ \sum_i y_i g(x_i) \\ \vdots \end{bmatrix}$$

Minimizing Sum of Squares = Finding Closest Ax in span(A)

- Compare two expressions we've derived: equal!

$$\begin{bmatrix} \sum_i f(x_i)f(x_i) & \sum_i f(x_i)g(x_i) & \cdots \\ \sum_i g(x_i)f(x_i) & \sum_i g(x_i)g(x_i) & \cdots \\ & \vdots & \end{bmatrix} \begin{bmatrix} a \\ b \\ \vdots \end{bmatrix} = \begin{bmatrix} \sum_i y_i f(x_i) \\ \sum_i y_i g(x_i) \\ \vdots \end{bmatrix}$$

Starting from goal of finding Ax in span(A) closest to b outside span(A)

$$\sum_i \begin{bmatrix} f(x_i) \\ g(x_i) \\ \vdots \end{bmatrix} \begin{bmatrix} f(x_i) \\ g(x_i) \\ \vdots \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} a \\ b \\ \vdots \end{bmatrix} = \sum_i y_i \begin{bmatrix} f(x_i) \\ g(x_i) \\ \vdots \end{bmatrix}$$

Starting from goal of minimizing sum of squares

Great, but how do we solve it?

Ways of Solving Linear Least Squares

$$\sum_i \begin{bmatrix} f(x_i) \\ g(x_i) \\ \vdots \end{bmatrix} \begin{bmatrix} f(x_i) \\ g(x_i) \\ \vdots \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} a \\ b \\ \vdots \end{bmatrix} = \sum_i y_i \begin{bmatrix} f(x_i) \\ g(x_i) \\ \vdots \end{bmatrix}$$

- Option 1:

  for each x_i, y_i

  compute $f(x_i)$, $g(x_i)$, etc.

  store in row i of A

  store y_i in b

  compute $(A^TA)^{-1} A^Tb$

- $(A^TA)^{-1} A^T$ is known as "pseudoinverse" of A

Ways of Solving Linear Least Squares

- Option 2:

  for each x_i, y_i

  compute $f(x_i)$, $g(x_i)$, etc.

  store in row i of A

  store y_i in b

  compute A^TA, A^Tb

  solve $A^TAx=A^Tb$

- Known as "normal equations" for least squares
  - Inefficient, since A typically larger than A^TA and A^Tb

Ways of Solving Linear Least Squares

- Option 3:

  for each x_i, y_i

  compute $f(x_i)$, $g(x_i)$, etc.

  accumulate outer product in U (= $A^T A$)

  accumulate product with y_i in v (= $A^T b$)

  solve Ux=v

$$\underbrace{\begin{bmatrix} \sum_i f(x_i)f(x_i) & \sum_i f(x_i)g(x_i) & \cdots \\ \sum_i g(x_i)f(x_i) & \sum_i g(x_i)g(x_i) & \cdots \\ & \vdots & \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} a \\ b \\ \vdots \end{bmatrix}}_{x} = \underbrace{\begin{bmatrix} \sum_i y_i f(x_i) \\ \sum_i y_i g(x_i) \\ \vdots \end{bmatrix}}_{v}$$

The Problem with Normal Equations

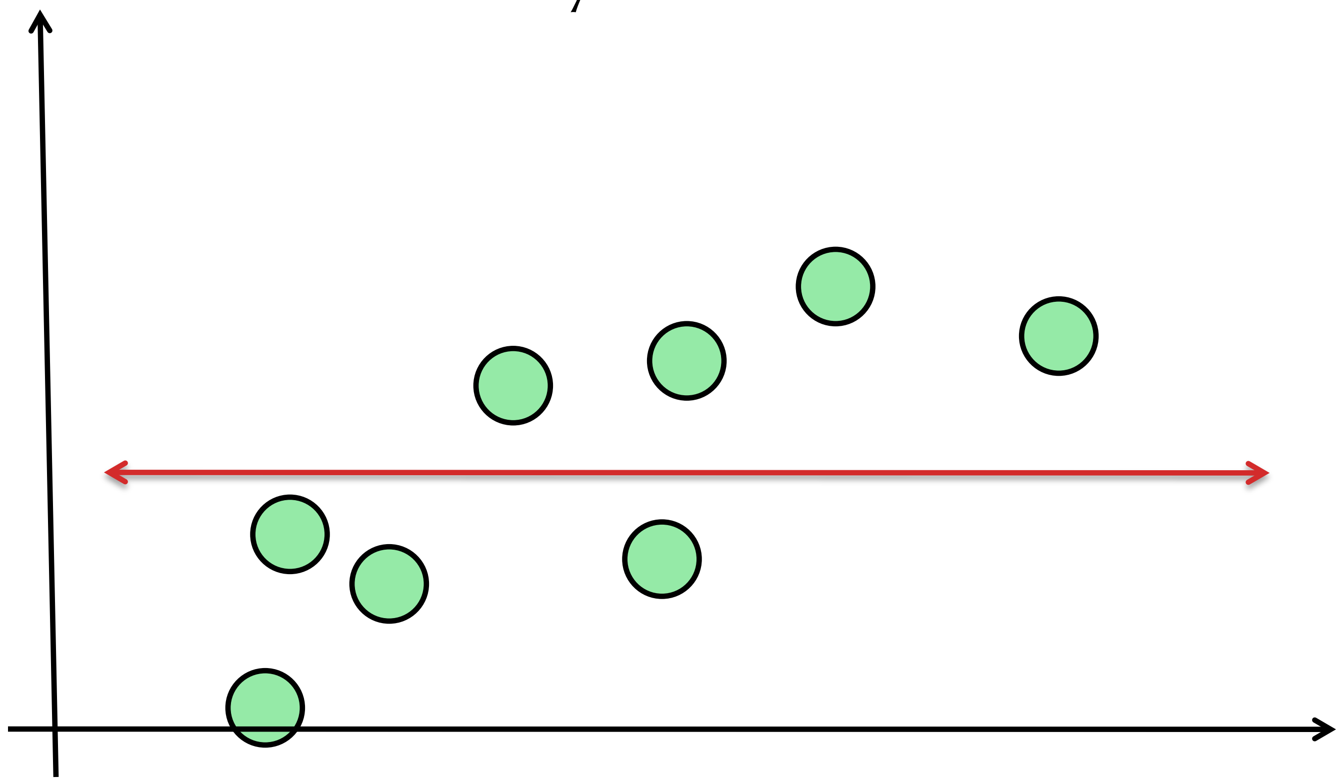
- Involves solving $\mathbf{A^T A x = A^T b}$
- This can be inaccurate
  - Independent of solution method
  - Remember: $$\frac{\|\Delta x\|}{\|x\|} \le cond(A)\frac{\|\Delta A\|}{\|A\|}$$
  - $\mathrm{cond}(A^T A) = [\mathrm{cond}(A)]^2$
- Next week: computing pseudoinverse stably
  - More expensive, but more accurate
  - Also allows diagnosing insufficient data

Special Cases

Special Case: Constant

- Let's try to model a function of the form

$$y = a$$



Special Case: Constant

- Let's try to model a function of the form

$$y = a$$

- Comparing to general form

$$y_i = af(\vec{x}_i) + bg(\vec{x}_i) + ch(\vec{x}_i) + \cdots$$

we have $f(x_i)=1$ and we are solving

$$\sum_i [1][a] = \sum_i [y_i]$$

$$\therefore \quad a = \frac{\sum_i y_i}{n}$$

Special Case: Line

- Fit to y=a+bx
- $f(x_i)=1$, $g(x_i)=x$. So, solve:

$$\sum_i \begin{bmatrix} 1 \\ x_i \end{bmatrix} \begin{bmatrix} 1 & x_i \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \sum_i y_i \begin{bmatrix} 1 \\ x_i \end{bmatrix}$$

$$(\mathbf{A}^{\mathrm{T}}\mathbf{A})^{-1} = \begin{bmatrix} n & \Sigma x_i \\ \Sigma x_i & \Sigma x_i^2 \end{bmatrix}^{-1} = \frac{\begin{bmatrix} \Sigma x_i^{\ 2} & -\Sigma x_i \\ -\Sigma x_i & n \end{bmatrix}}{n\Sigma x_i^{\ 2} - (\Sigma x_i)^2}, \quad \mathbf{A}^{\mathrm{T}} b = \begin{bmatrix} \Sigma y_i \\ \Sigma x_i y_i \end{bmatrix}$$

$$a = \frac{\Sigma x_i^{\ 2}\, \Sigma y_i - \Sigma x_i\, \Sigma x_i y_i}{n\Sigma x_i^{\ 2} - (\Sigma x_i)^2}, \quad b = \frac{n\,\Sigma x_i y_i - \Sigma x_i\, \Sigma y_i}{n\Sigma x_i^{\ 2} - (\Sigma x_i)^2}$$

Variant: Weighted Least Squares

Weighted Least Squares

- Common case: the (x_i, y_i) have different uncertainties associated with them
- Want to give more weight to measurements of which you are more certain
- Weighted least squares minimization

$$\min \chi^2 = \sum_i w_i \left(y_i - f(x_i)\right)^2$$

- If "uncertainty" (stdev) is σ, best to take $w_i = 1/\sigma_i^2$

Weighted Least Squares

- Define weight matrix W as

$$\mathbf{W} = \begin{pmatrix} w_1 & & & & 0 \\ & w_2 & & & \\ & & w_3 & & \\ & & & w_4 & \\ 0 & & & & \ddots \end{pmatrix}$$

- Then solve weighted least squares via

$$\mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{A}\,x = \mathbf{A}^{\mathrm{T}}\mathbf{W}\,b$$

Understanding Error and Uncertainty

Error Estimates from Linear Least Squares

- For many applications, finding model is useless without estimate of its accuracy
- Residual is b – Ax
- Can compute $\chi^2 = (b - Ax) \cdot (b - Ax)$
- How do we tell whether answer is good?
  - Lots of measurements
  - χ^2 is small
  - χ^2 increases quickly with perturbations to x ($\rightarrow$ **standard variance** of estimate is small)

Error Estimates from Linear Least Squares

- Let's look at increase in χ^2:

$$
\begin{gathered}
x \to x + \delta x \\
\left(b - \mathbf{A}(x + \delta x)\right)^{\mathrm{T}} \left(b - \mathbf{A}(x + \delta x)\right) \\
= \left((b - \mathbf{A}x) - \mathbf{A}\delta x\right)^{\mathrm{T}} \left((b - \mathbf{A}x) - \mathbf{A}\delta x\right) \\
= (b - \mathbf{A}x)^{\mathrm{T}}(b - \mathbf{A}x) - 2\delta x^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}(b - \mathbf{A}x) + \delta x^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}\mathbf{A}\delta x \\
= \chi^2 - 2\delta x^{\mathrm{T}}(\mathbf{A}^{\mathrm{T}}b - \mathbf{A}^{\mathrm{T}}\mathbf{A}x) + \delta x^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}\mathbf{A}\delta x \\
\text{So, } \chi^2 \to \chi^2 + \delta x^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}\mathbf{A}\delta x
\end{gathered}
$$

- So, the *bigger* A^TA is, the *faster* error increases as we move away from current x

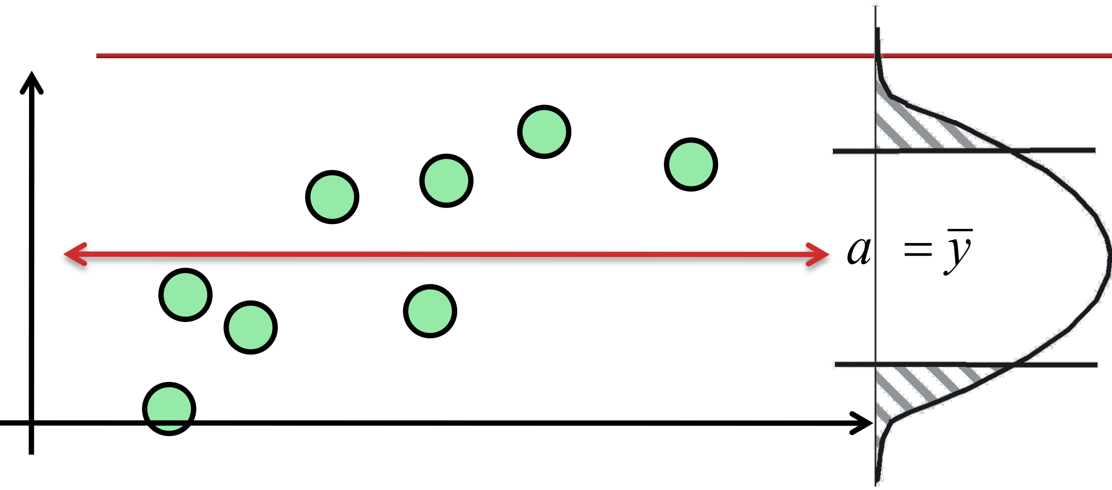
Error Estimates from Linear Least Squares

- $C=(A^TA)^{-1}$ is called *covariance* of the data
- The "**standard variance**" in our estimate of x is

$$\sigma^2 = \frac{\chi^2}{n-m}\mathbf{C}$$

- This is a matrix:
  - Diagonal entries give variance of estimates of components of x: e.g., var(a_0)
  - Off-diagonal entries explain mutual dependence: e.g., cov(a_0, a_1)
- n–m is (# of samples) minus (# of degrees of freedom in the fit): consult a statistician…

Special Case: Error in Constant Model



$$\chi^2 = \sum_i (y_i - a)^2$$

$$\mathbf{C} = \left[\frac{1}{n}\right]$$

$$\text{standard deviation of data}: \sigma = \sqrt{\frac{\sum_i (y_i - a)^2}{n-1}}$$

$$\text{standard error of a}: \sigma_a = \underbrace{\sqrt{\frac{\sum_i (y_i - a)^2}{n-1}} \Big/ \sqrt{n}}$$

"standard deviation of mean"

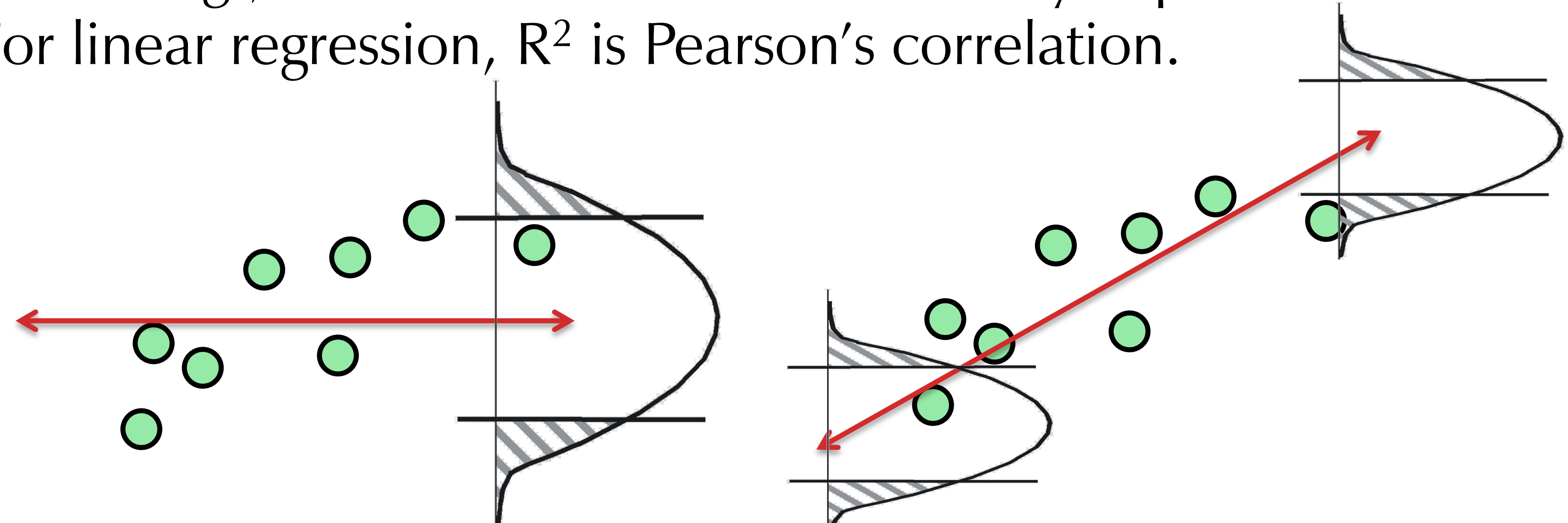
Coefficient of Determination

$$R^2 \equiv 1 - \frac{\chi^2}{\sum_i (y_i - \bar{y})^2}$$

R^2 : Proportion of observed variability that is explained by the model (vs. just the mean)

e.g., $R^2 = 0.7$ means 70% variability explained

For linear regression, R^2 is Pearson's correlation.



Keep in mind…

- In general, uncertainty in estimated parameters goes down slowly: like 1/sqrt(# samples)
- Formulas for special cases (like fitting a line) are messy: simpler to think of $A^TAx=A^Tb$ form
- Normal equations method often not numerically stable: orthogonal decomposition methods used instead
- Linear least squares is not always the most appropriate modeling technique…

Next time

- Non-linear models
  - Including logistic regression
- Dealing with outliers and bad data
- Practical considerations
  - Is least squares an appropriate method for my data?